AIChE
American Institute of Chemical Engineers
Netherlands/ Belgium Section

Mobatec
model-based technology

Process Modelling Made Easy !

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Mobatec
MODELLER

Free Demo

The **free** demo-version of Mobatec Modeller includes **Examples** and **Learning Modules.**

Go to **www.mobatec.nl** and download it for free!

Mobatec | Modelling Examples | Modelling Approaches | Our Approach | Examples | Conclusions

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Presentation Overview

Overview

- Company Overview
- Modelling Examples
  - Application Areas
  - Specific Issues
- Modelling Approaches
  - Methodologies
  - Modelling Wisdom
- Mobatec Approach
- Examples / Demonstration
- Conclusions

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Specialisation
Expertise
Main Services and Products
Why Mobatec Modeller?
Why Modelling?

Specialisation

- Mathematical Modelling of any kind of process knowledge in Chemical Engineering

- Modelling Activities for purpose of:
  - Process Design
  - **Process Analysis**
  - Process Optimisation
  - Process Control
  - **Real-Time Training Simulation**

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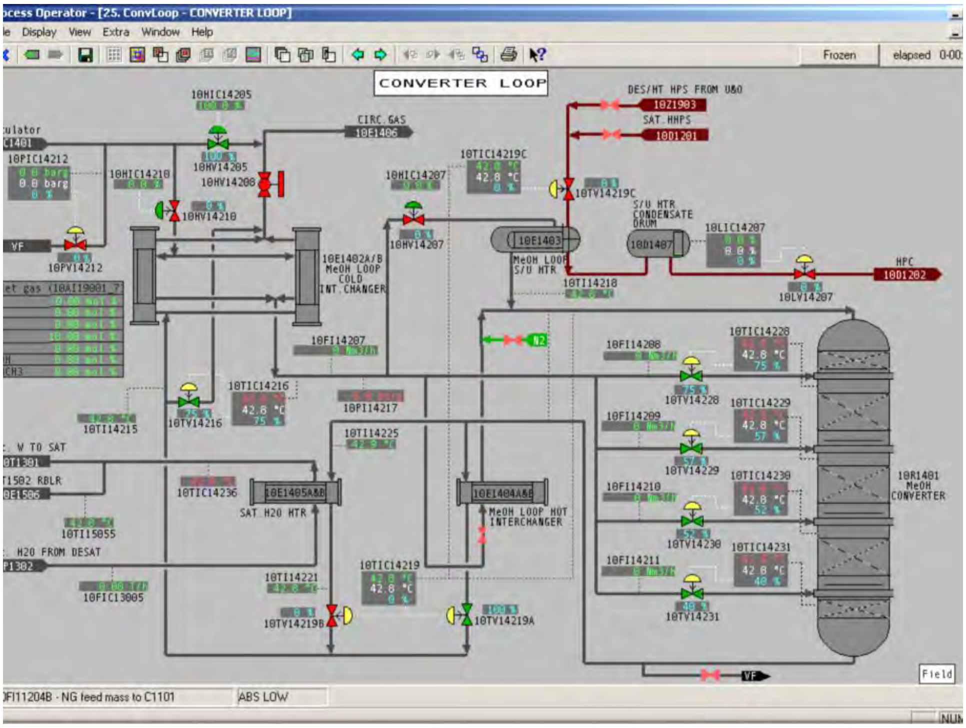

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- Specialisation
- Expertise
- Main Services and Products
- Why Mobatec Modeller?
- Why Modelling?

Expertise

- Evaporation
- Polymers
- Crystallisation
- Thermodynamics
- Numerical Mathematics
- Software Development of Modelling Tools
  - Solver for large sets of differential and algebraic equations
  - Modelling Environment
  - Parameter Estimation
  - Data Reconciliation
- Reactor Modelling
  - Homogeneous systems
  - Heterogeneous systems
- Distillation
- Stripping
- Heat and Mass Transfer
  - Vapour/Liquid interface
  - Transfer from bulk fluid to particles
  - Pore diffusion
  - Adsorption on catalyst surface
  - Multi-phase interactions

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Main Services and Products

- Construction of Process Models
- Consulting Services Related to Mathematical Modelling
- Mobatec Modeller
- LauTrane Solver

Modelling can be Easy !

Mobatec Modeller builds on a structured modelling methodology.

*It is **our goal** to bring this easy to grasp modelling methodology to the world and to teach engineers that modelling can actually be quite easy and very valuable.*

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Some of the Mobatec customers:

STC-GROUP
DSM
AVEBE
سابك sabic
HUNTSMAN
TU/e Technische Universiteit Eindhoven University of Technology
bodec
nyrstar
Protomation
ExplainMedia
lyondellbasell
Stamicarbon pure knowledge
ACTEMIUM

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- Specialisation
- Expertise
- Main Services and Products
- Why Mobatec Modeller?
- Why Modelling?

Why Mobatec Modeller?

- Time spent on modelling often greater than time needed for finding solution
- Higher complexity of models
- Assist in model building
- Reduce time effort
- Reduce low-level modelling errors
- Provide input for existing simulators
- Increase maintainability of models
  - ✓ Models also understandable by persons who did not develop the model

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Specialisation
Expertise
Main Services and Products
Why Mobatec Modeller?
Why Modelling?

Why Modelling?

- Control
- Design
- Simulation
- Optimization
- Etc.

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Specialisation
Expertise
Main Services and Products
Why Mobatec Modeller?
Why Modelling?

Application Areas

- Process design
- Process control and diagnosis / PLC testing
- Troubleshooting
- Process safety
- Optimization
- Operator training / Real time simulation
- Research
- Engineering
- Environmental impact assessment

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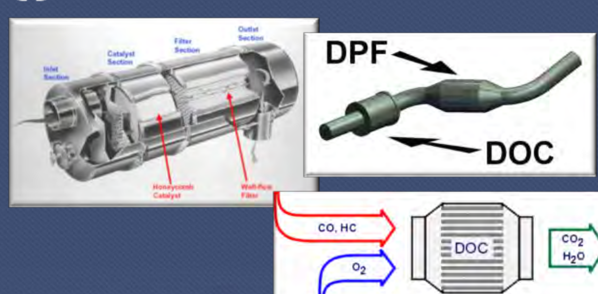
Application Areas
Examples
Operator Training Simulator

Diesel Oxidation Catalyst



Model features:

- Complex reaction scheme and reaction kinetics
- Validated model against pilot data
- Distributed parameter model

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Safety and Risk Assessment (BLEVE Radiation)

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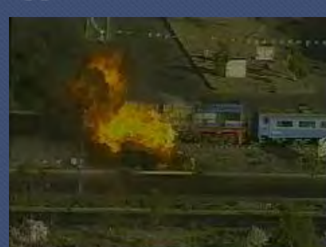
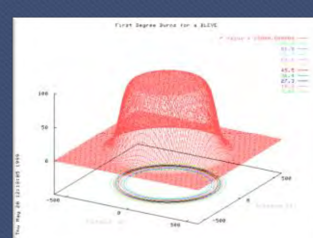
Application Areas
Examples
Operator Training Simulator

Safety and Risk Assessment (BLEVE Radiation)





3D surface showing percent first degree burns for a BLEVE

Model features:

- Empirical model based on field trials and actual explosion effects
- BLEVE size and duration computed
- Resource vulnerability based on stochastic (Probit) model

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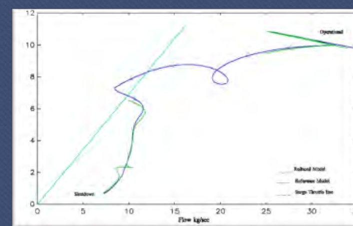
Application Areas
Examples
Operator Training Simulator

Surge Control Design for a Hydrogen Compressor



Head (bar) versus flowrate (kg/s) during controlled shutdown

Model features:

- Process model plus control elements considered

- Complex nonlinear dynamics and potential discontinuous behaviour

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Application Areas
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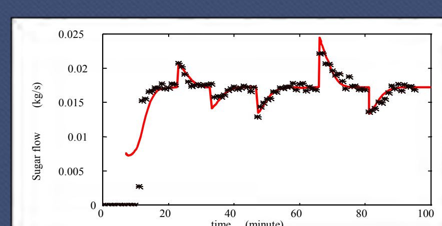
Sugar Drying Control



Sugar flowrate versus time under startup and airflow changes

Model features:

- Grey-box model based on mass & heat transfer combined with particle transport

- Validated model against pilot plant data

- Provides basis for model-based control system design

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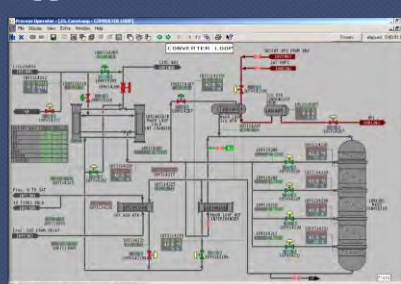
Wastewater Treatment

- Activated sludge process
- Clarification
- Process control

Model features:

- Complex biological reactions within a mechanistic model
- Validation against plant data challenging
- Provides basis for model-based plant and control system design

Operator Training Simulator



- Large Dynamics Models
- Process control
- Disturbances

Model features:

- Physical model of entire production plant
- Should be able to predict from startup to 100% load, within desired accuracy
- Provides basis for model-based plant and control system design

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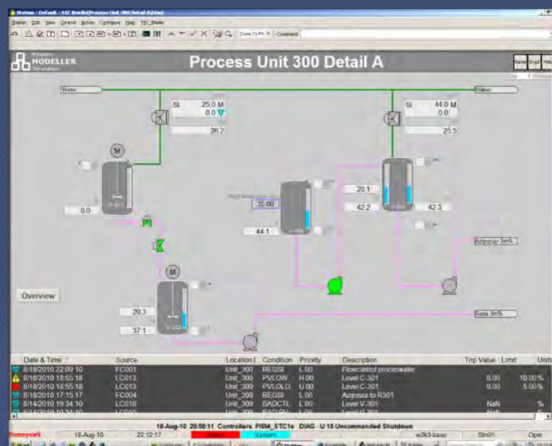
Operator Training Simulator



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Application Areas
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Application Areas
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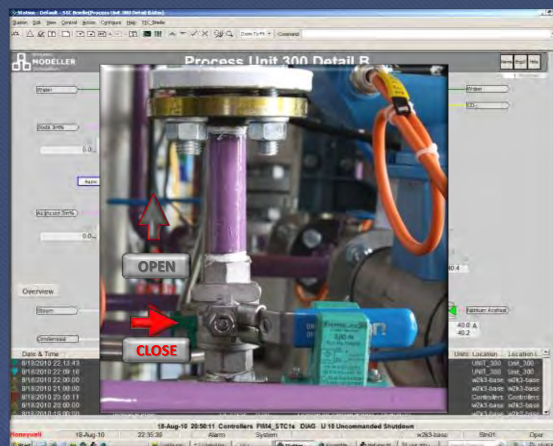

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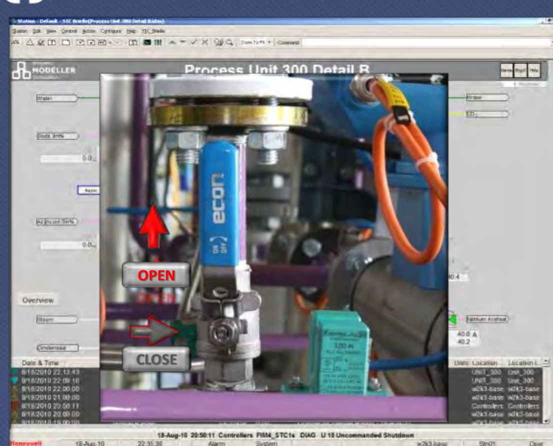

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VR DEMO - Not for Resale - Operator 1
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REGENERATOR & REACTOR/STRIPPER
FRACTIONATION
FURNACE & OVERHEAD
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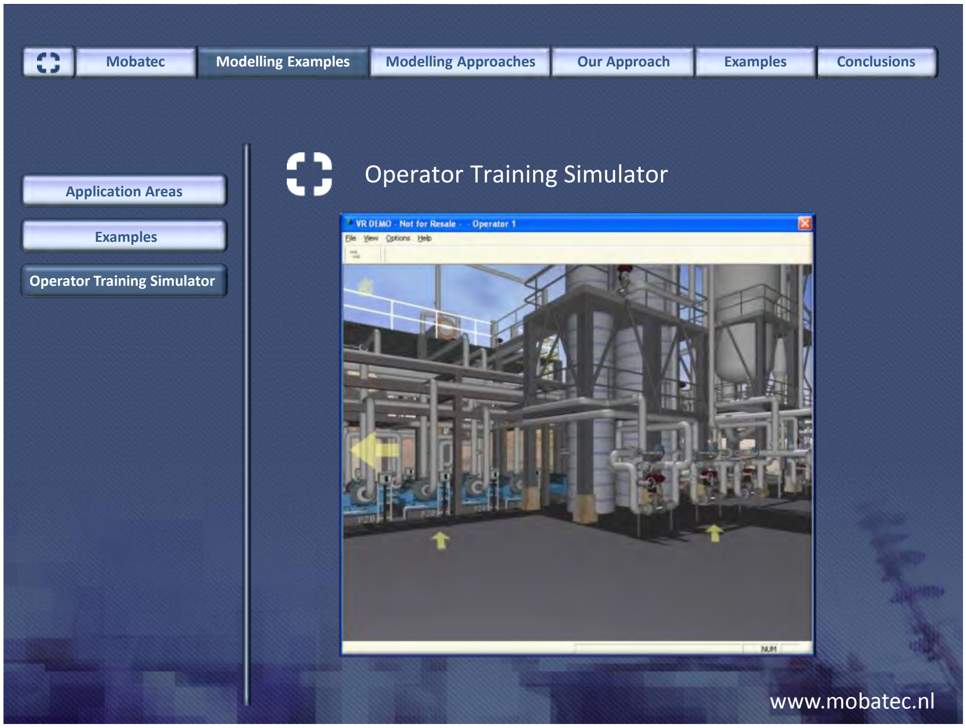
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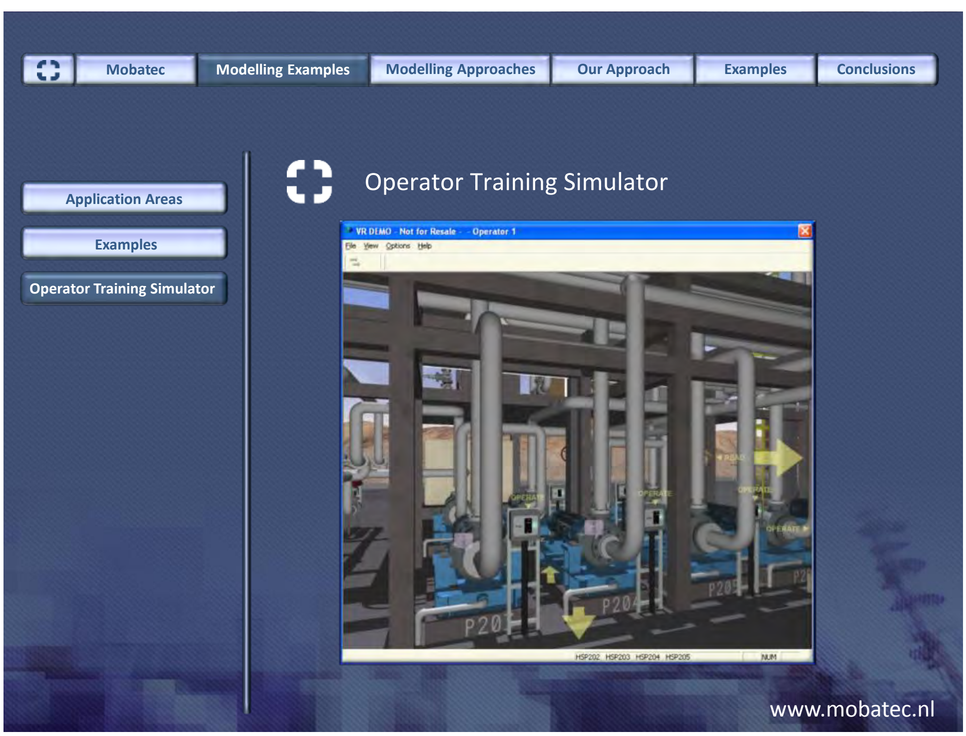
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- Application Areas
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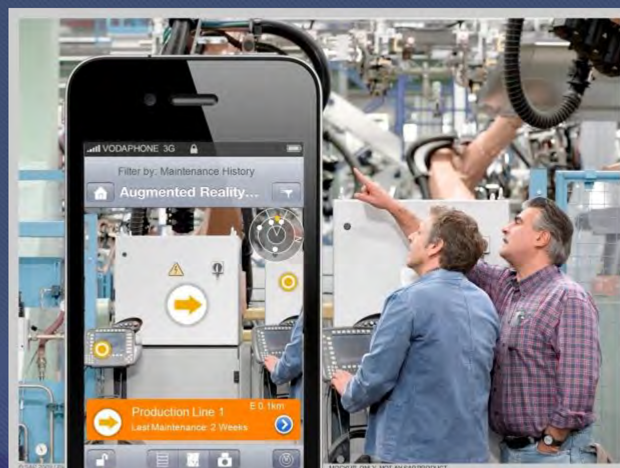
- Operator Training Simulator

Augmented Reality



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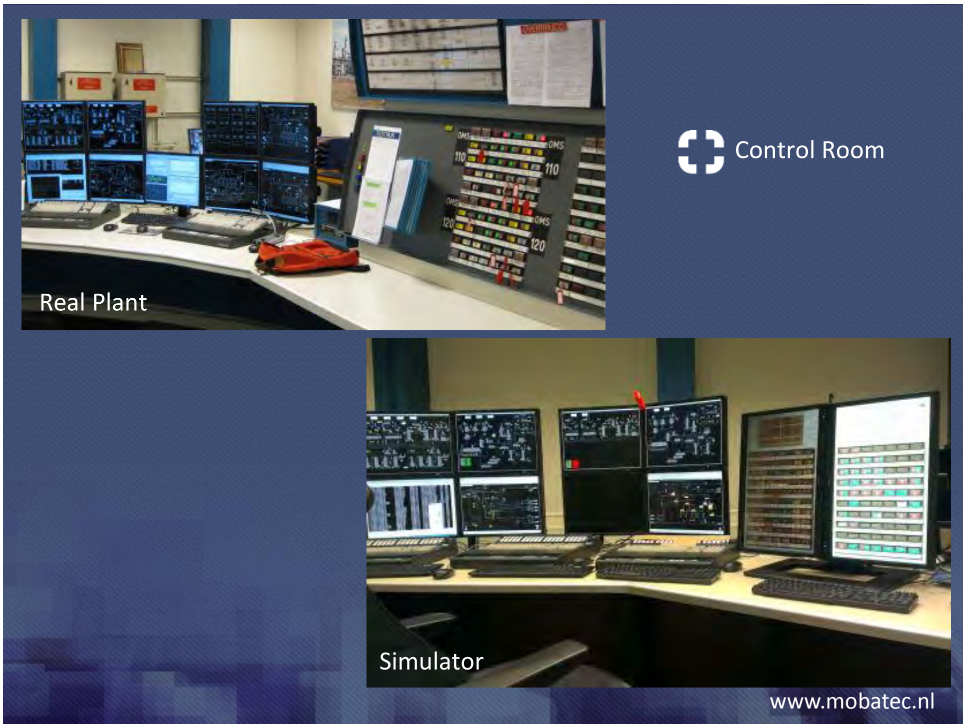
Real Plant
Control Room
Simulator
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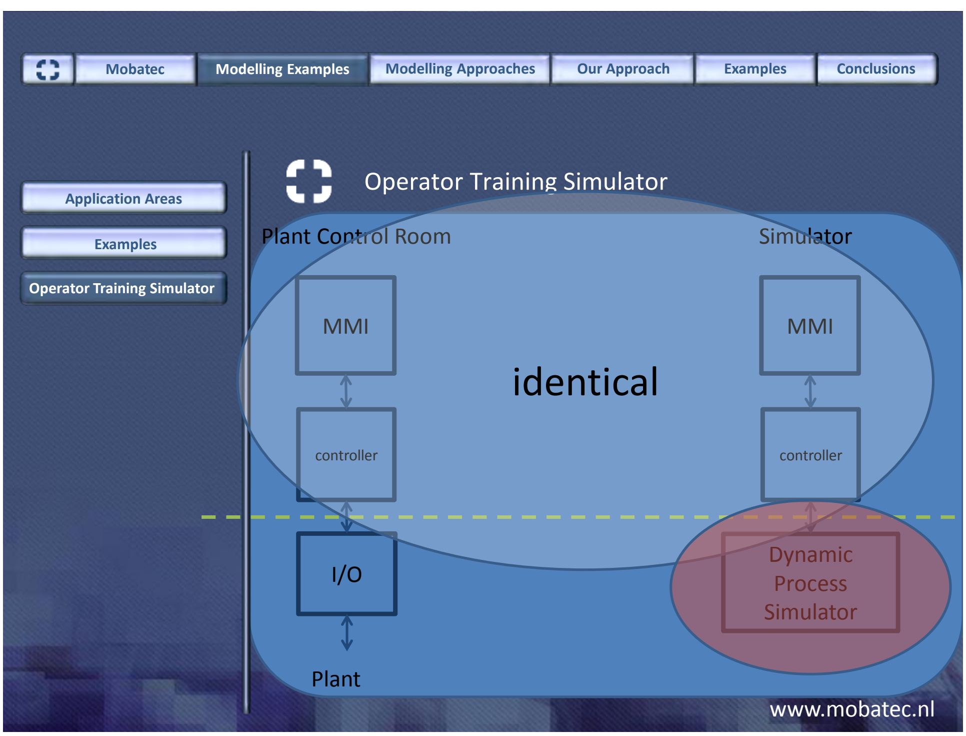
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Operator Training Simulator
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controller
I/O
Dynamic
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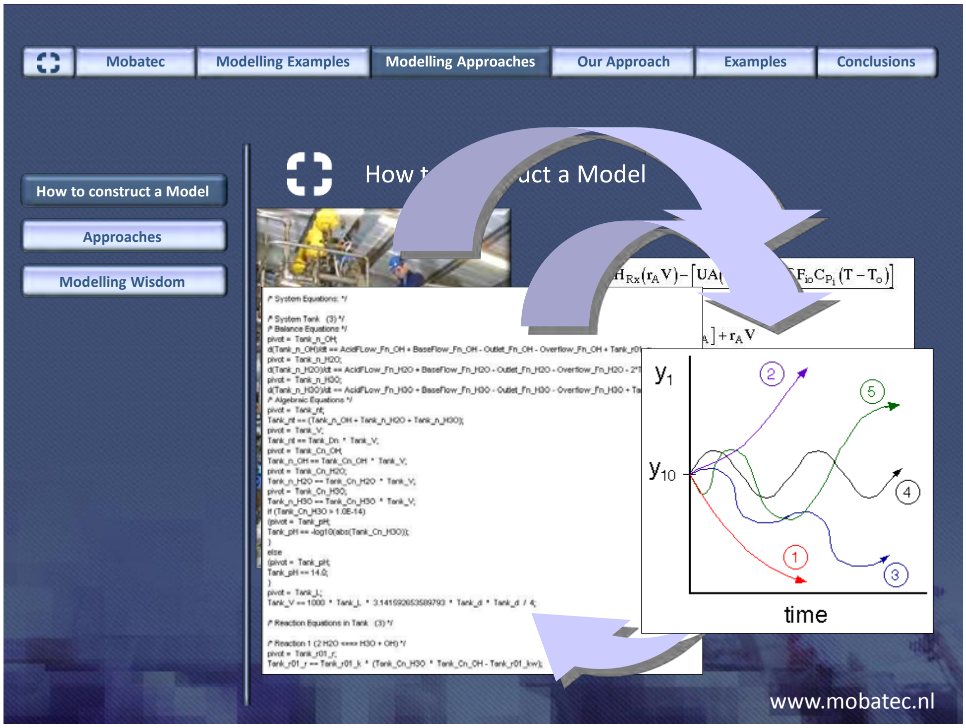
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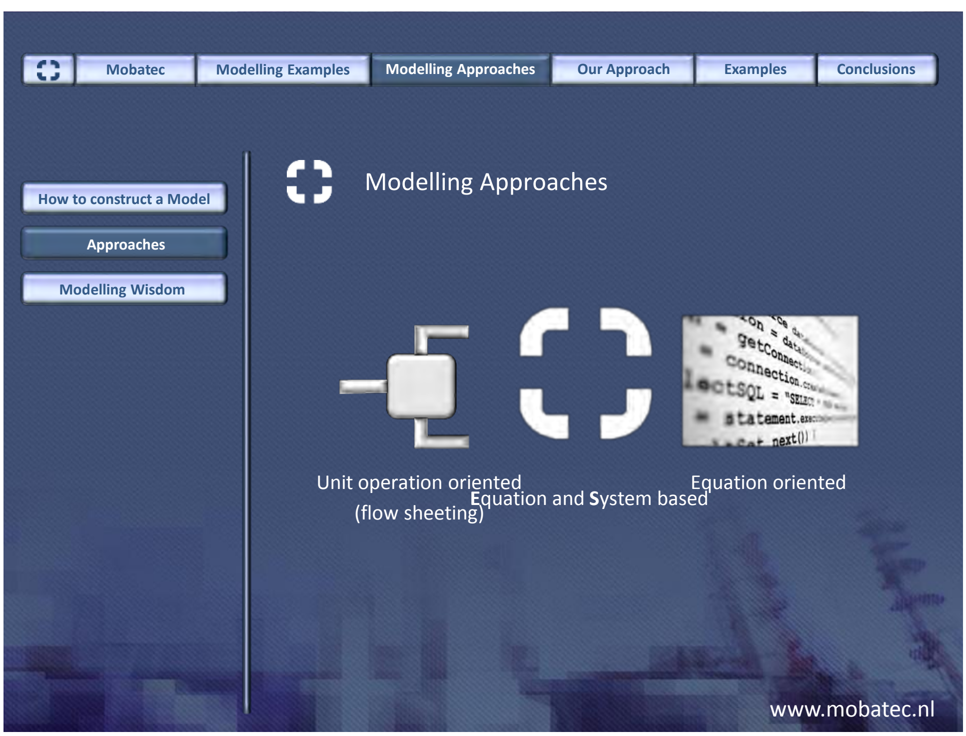
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Modelling Approaches
Unit operation oriented
(flow sheeting)
Equation and System based
Equation oriented
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Modelling Approaches (1)

Unit operation oriented / flow sheeting:

- Steady state modelling
- Mass and energy balances for free
- Configuration of predefined unit operations
- Inflexible when user models are to be created
- Sequential local solving of units (recycle problem)
- No problems with Degrees Of Freedom (DOF)

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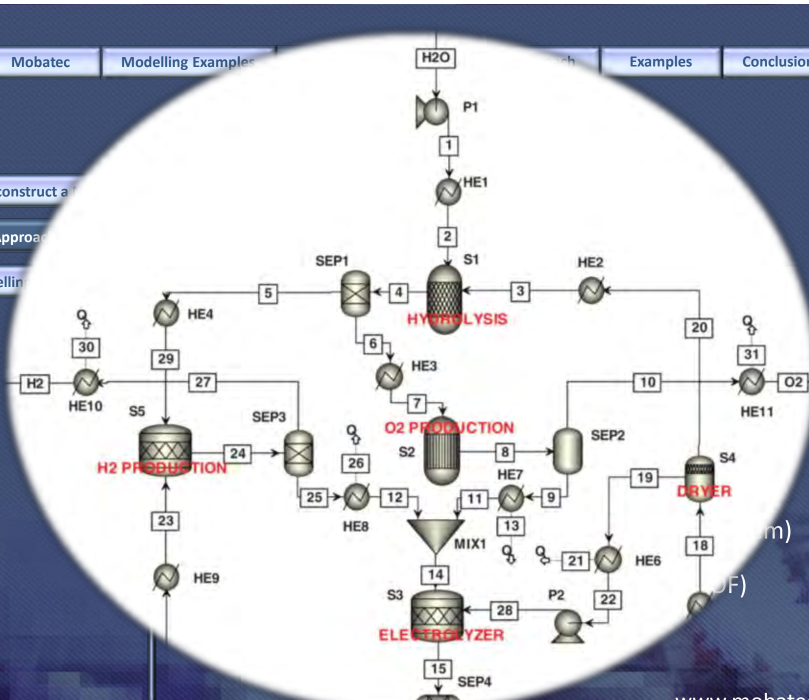

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How to construct a Model

Approaches

Modelling Wisdom

Modelling Approaches (2)

Equation oriented

- Dynamic modelling
- Mass and energy balances to be coded
- Few options for predefined unit operations
- Flexible when user models are to be created
- Implicit global solving of units (no recycle problem)
- Problems with DOF of model
- Problems with initialization of model

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How to construct a Mo

Approaches

Modelling Wisd

```
pivot = Dm_P110_Suction;
Dm_P110_Suction * Vn_P110_Suction == MW_P110_Suction;
pivot = V_P110_Suction;
V_P110_Suction == Vn_P110_Suction * nt_P110_Suction;
if (V_P110_Suction > V0_P110_Suction)
{pivot = P_P110_Suction;
P_P110_Suction == P0_P110_Suction + Pfac * (V_P110_Suction - V0_P110_Suction) / V0_P110_Suction;
}
else
{pivot = P_P110_Suction;
P_P110_Suction == P0_P110_Suction;
}
THERMO_SPECIES_IDS = 1, 138;
THERMO_FRACTIONS = $Xn_EB_P110_Suction;
THERMO_FUGC = $THERMO_DUMMY;
pivot = 0, T_P110_Suction, Vn_P110_Suction;
Thermo_2(THERMO_FUGC, Hn_P110_Suction, Vn_P110_Suction, THERMO_SPECIES_IDS, T_P110_Suction, P_P110_Suction,
THERMO_FRACTIONS, THERMO_LIQ, THERMO_FLAGS_Liquid);

/* System P110_Discharge   (1.10.2) */
/* Balance Equations */
pivot = n_EB_P110_Discharge;
d(n_EB_P110_Discharge)/dt == Fn_EB_P110_Pump - Fn_EB_L106;
pivot = H_P110_Discharge;
d(H_P110_Discharge)/dt == HF_P110_Pump - Q_P110_h0038 + Wdis_P110_Pump - HF_L106;
/* Algebraic Equations */
pivot = nt_P110_Discharge;
nt_P110_Discharge == (n_EB_P110_Discharge);
pivot = Xn_EB_P110_Discharge;
n_EB_P110_Discharge == Xn_EB_P110_Discharge * nt_P110_Discharge;
pivot = Hn_P110_Discharge;
H_P110_Discharge == Hn_P110_Discharge * nt_P110_Discharge;
;
;
pivot = V_P110_Discharge;
V_P110_Discharge == Vn_P110_Discharge * nt_P110_Discharge;
if (V_P110_Discharge > V0_P110_Discharge)
{pivot = P_P110_Discharge;
P_P110_Discharge == P0_P110_Discharge + Pfac * (V_P110_Discharge - V0_P110_Discharge) / V0_P110_Discharge;
}
else
{pivot = P_P110_Discharge;
P_P110_Discharge == P0_P110_Discharge;
}
THERMO_SPECIES_IDS = 1, 138;
THERMO_FRACTIONS = $Xn_EB_P110_Discharge;
THERMO_FUGC = $THERMO_DUMMY;
pivot = 0, T_P110_Discharge, Vn_P110_Discharge;
Thermo_2(THERMO_FUGC, Hn_P110_Discharge, Vn_P110_Discharge, THERMO_SPECIES_IDS, T_P110_Discharge,
P_P110_Discharge, THERMO_FRACTIONS, THERMO_LIQ, THERMO_FLAGS_Liquid);
```

m)

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How to construct a Model

Approaches

Modelling Wisdom

Modelling Approaches (3)

Equation and system based

- Dynamic modelling
- Mass and energy balances for free
- Library of equations
- Easy extendable libraries for predefined unit operations
- Flexible when user models are to be incorporated
- No problems with DOF systems
- No problems with initialization per system

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How to construct a Model
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Modelling Wisdom

Modelling Wisdom

- Modelling is a tool no goal in itself
- Universal models are uneconomical
- Complexity of model should be in line with goal

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How to construct a Model
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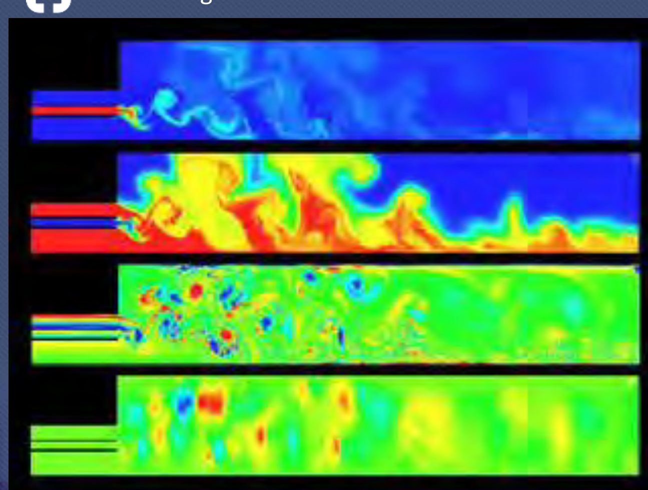
Modelling Wisdom

Modelling Wisdom



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Modelling Wisdom

- Modelling is a tool no goal in itself
- Universal models are uneconomical
- Complexity of model should be in line with goal
- A model can not explain more than it contains

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How to construct a Model
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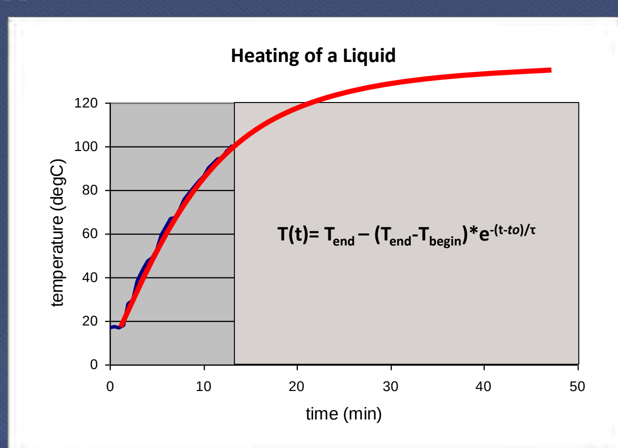
Modelling Wisdom

Modelling Wisdom



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How to construct a Model
Approaches
Modelling Wisdom

Modelling Wisdom

- Be aware of the model's purpose
- Be aware of the model's assumptions
- Be aware of the model's operating window
- "Garbage in, garbage out"
- Modelling is the art of leaving out

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How to construct a Model
Approaches
Modelling Wisdom

Modelling Wisdom

"All models are wrong ….
…. some are useful !"

… George Box

"Models should be as simple as possible …
…. but not simpler !"

… Albert Einstein

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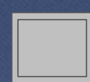
Physical Topology
Examples
Species Topology
Equation Topology
Dynamic Equations
Classes of Relations
Model Equations
Algebraic Equations

Modelling Methodology: Step 1

Physical Topology

- “Break down” process into smaller, interconnected parts.
- Two basic building blocks



Elementary Systems

Connections

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Physical Topology
Examples
Species Topology
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Physical Topology Example 1

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- Physical Topology
  - Examples
- Species Topology
- Equation Topology
- Dynamic Equations
- Classes of Relations
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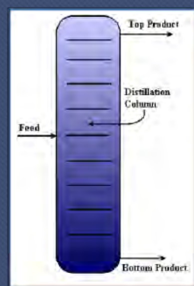
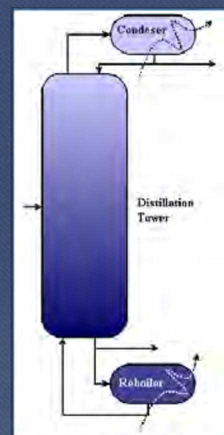
- Algebraic Equations

Physical Topology Example 1





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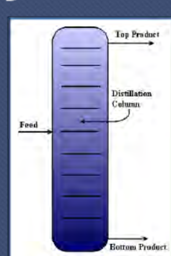
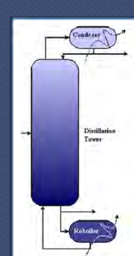
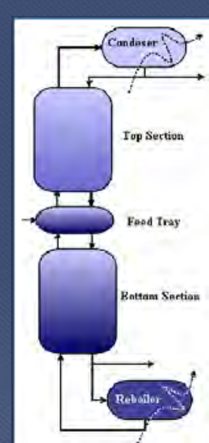
Physical Topology Example 1







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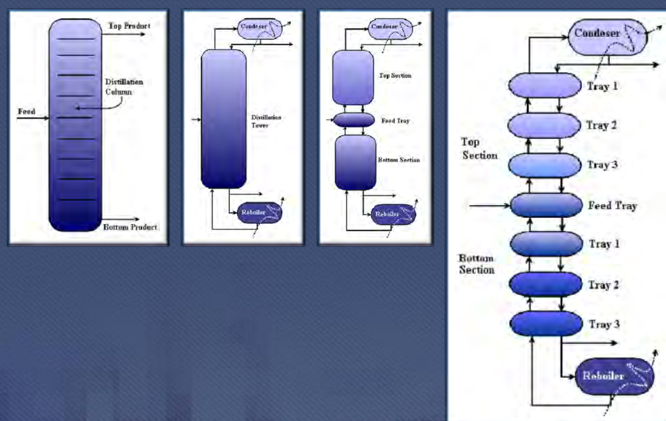
Physical Topology Example 1



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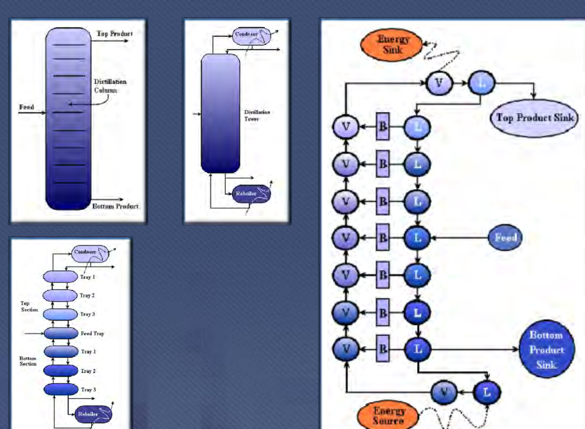
Physical Topology Example 1



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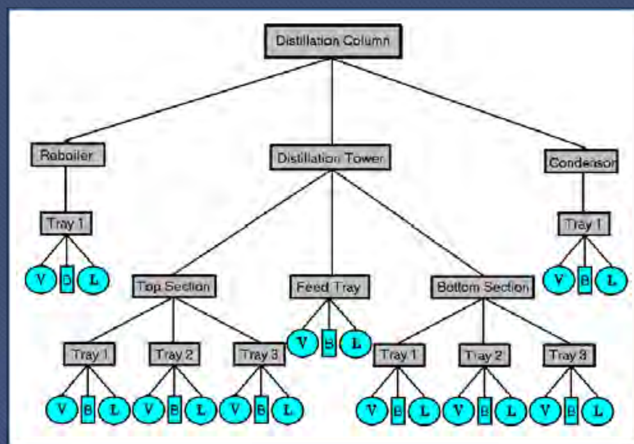
Physical Topology Example 1



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Physical Topology
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Modelling Methodology: Step 2

Species Topology

- Define “Chemistry” of process

Example:

Species and Reactions in System:

H_2O – Water
CH_4 – Methane
O_2 – Oxigen
N_2 – Nitrogen
CO_2 – Carbon Dioxide

$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O$

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Modelling Methodology: Step 3

Equation Topology

- Information of *Physical Topology* and *Species Topology* .

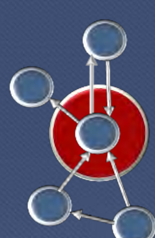
Generating balance equations is trivial !

(Automated by Mobatec Modeller)

- Define details, i.e. the *Constitutive Equations*: Select equations for transfer laws, kinetics, geometry, equations of state, etc. from (extensible) database.

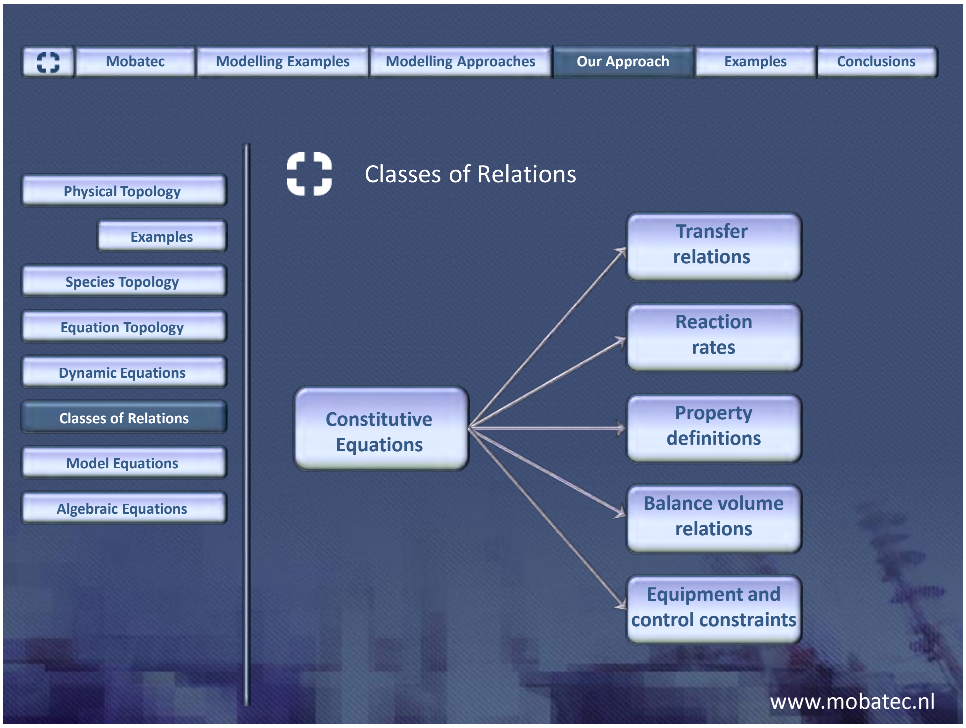
- Important for model completion: consistent set of equations and consistent initial values.

Dynamic Equations



- **System:** capacitive element
- **State of system:** set of fundamental extensive quantities
- **Fundamental Extensive Quantity Φ:** system property for which conservation and superposition principles applies
- **Conservation Principle:**

Acc = In – Out + Prod - Cons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Balance volume relations
Equipment and control constraints
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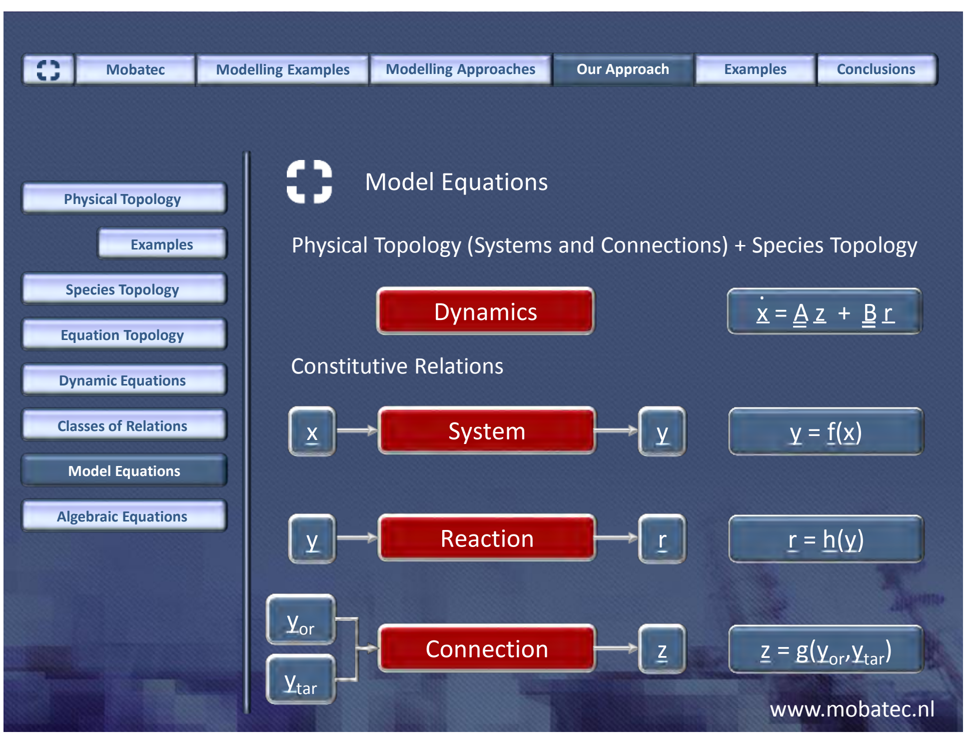
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Physical Topology (Systems and Connections) + Species Topology
Dynamics
$\underline{\dot{x}} = \underline{\underline{A}}\,\underline{z} + \underline{\underline{B}}\,\underline{r}$
Constitutive Relations
$\underline{x}$
System
$\underline{y}$
$\underline{y} = \underline{f}(\underline{x})$
$\underline{y}$
Reaction
$\underline{r}$
$\underline{r} = \underline{h}(\underline{y})$
$\underline{y}_{or}$
$\underline{y}_{tar}$
Connection
$\underline{z}$
$\underline{z} = \underline{g}(\underline{y}_{or}, \underline{y}_{tar})$
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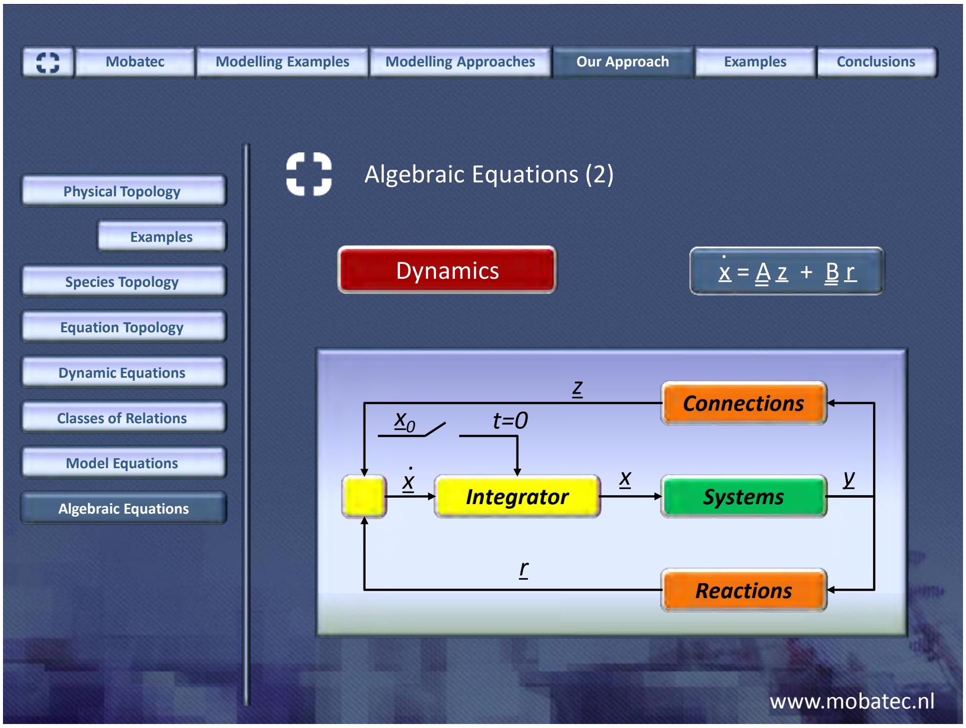

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Algebraic Equations (2)
Dynamics
$\dot{\underline{x}} = \underline{A}\,\underline{z} + \underline{B}\,\underline{r}$
$\underline{z}$
Connections
$\underline{x}_0$
t=0
$\dot{\underline{x}}$
Integrator
$\underline{x}$
Systems
$\underline{y}$
$\underline{r}$
Reactions
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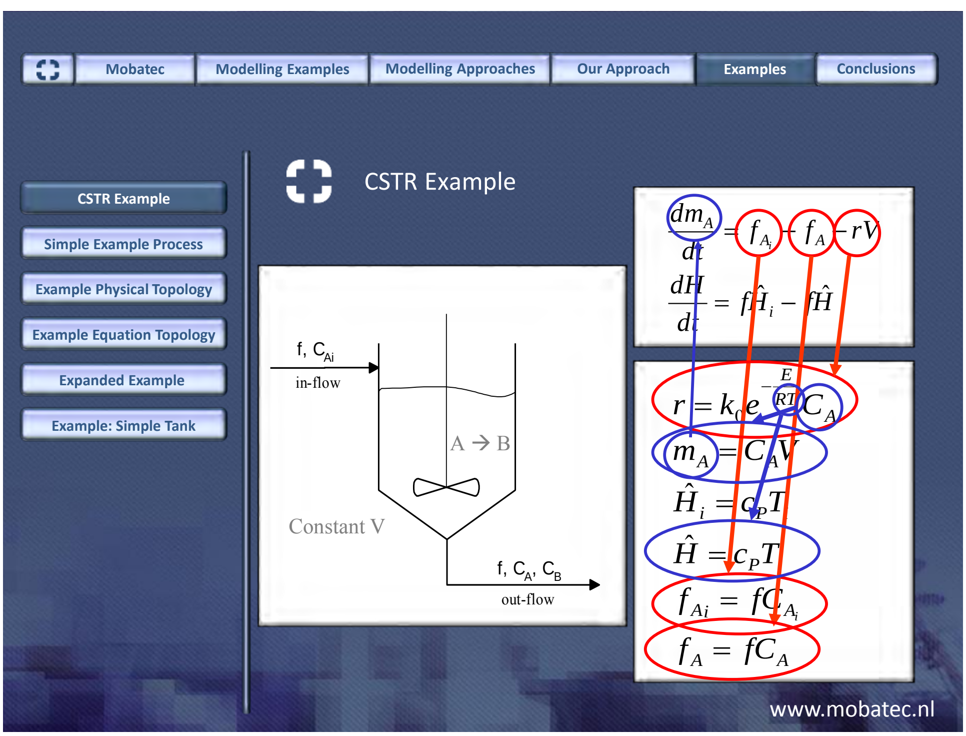

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Example: Simple Tank
CSTR Example
f, C_{Ai}
in-flow
A → B
Constant V
f, C_A, C_B
out-flow
$\frac{dm_A}{dt} = f_{A_i} - f_A - rV$
$\frac{dH}{dt} = f\hat{H}_i - f\hat{H}$
$r = k_0 e^{-\frac{E}{RT}} C_A$
$m_A = C_A V$
$\hat{H}_i = c_P T$
$\hat{H} = c_P T$
$f_{Ai} = fC_{A_i}$
$f_A = fC_A$
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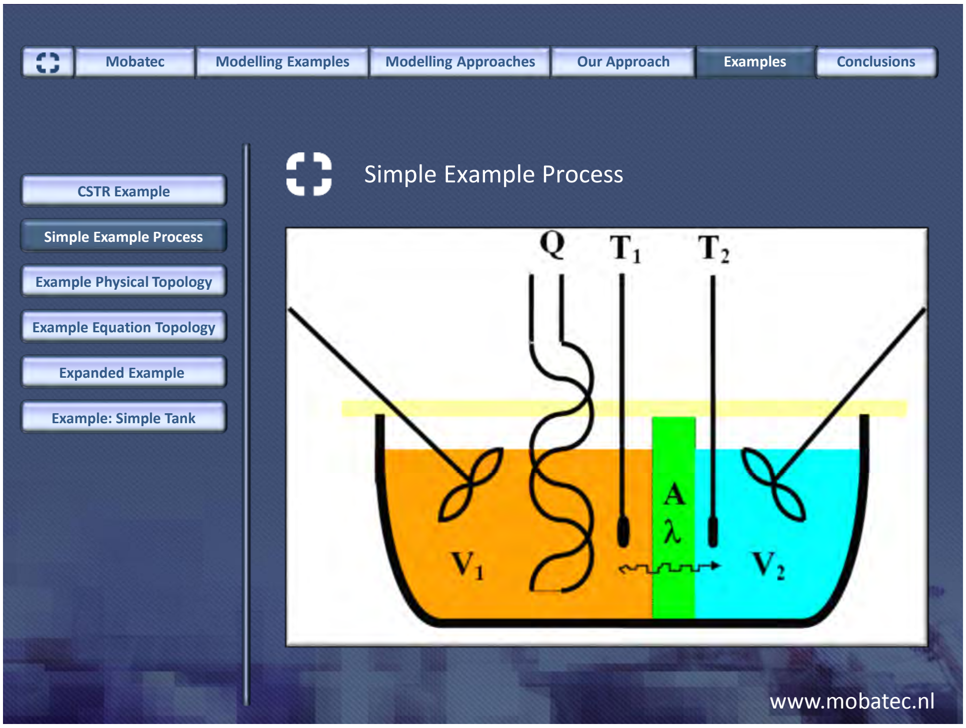
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Q
T1
T2
A
λ
V1
V2
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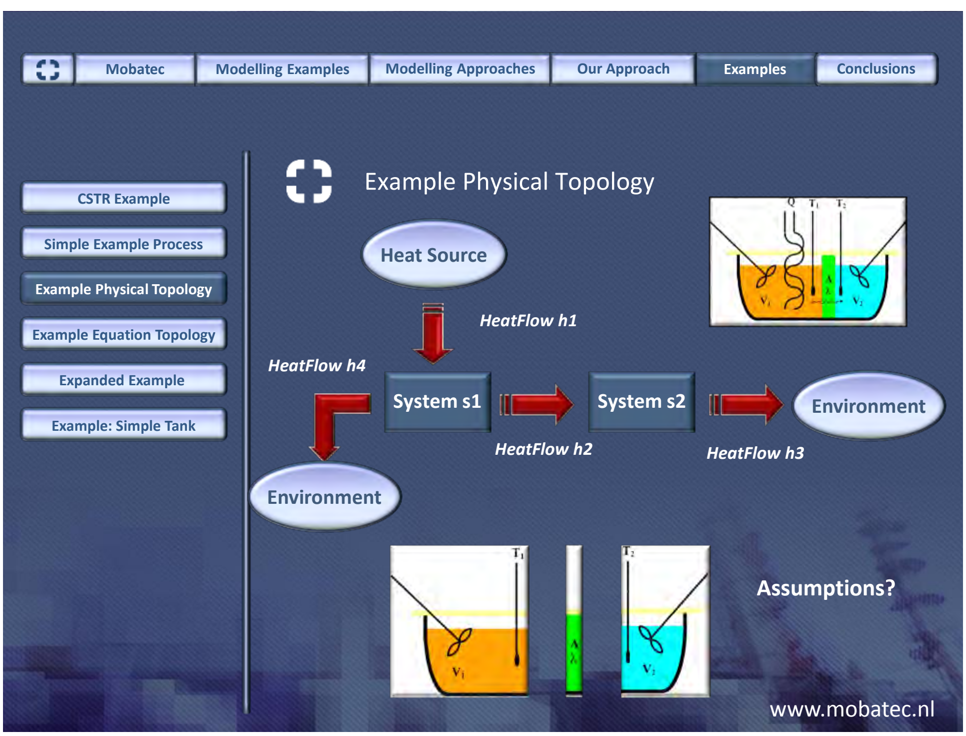
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Heat Source
HeatFlow h1
HeatFlow h4
System s1
System s2
Environment
HeatFlow h2
HeatFlow h3
Environment
Assumptions?
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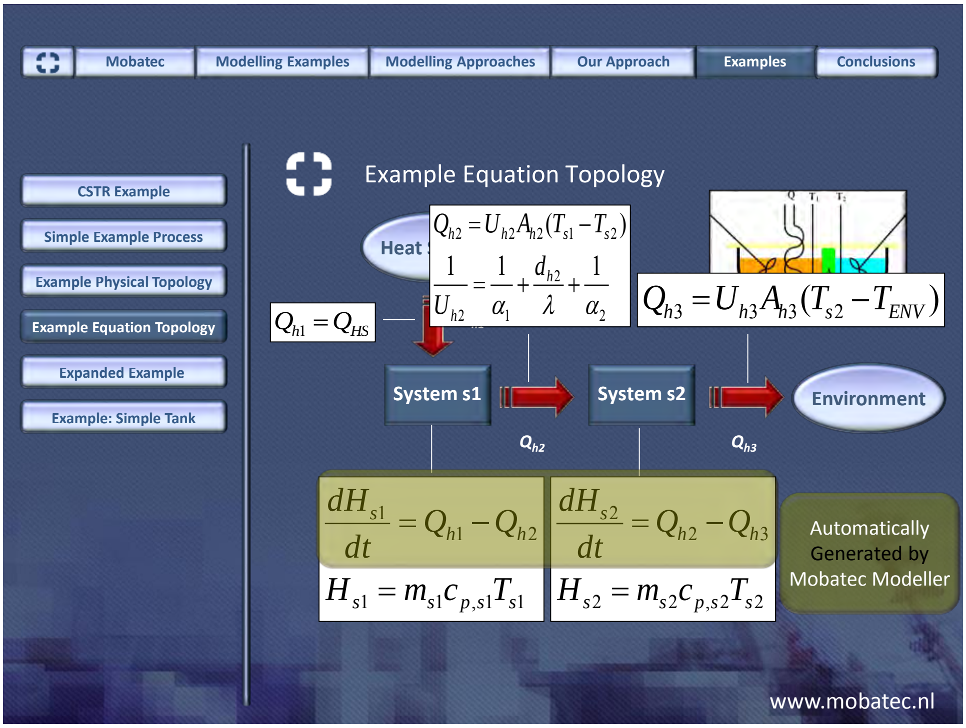
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Heat
$Q_{h2} = U_{h2} A_{h2} (T_{s1} - T_{s2})$
$\frac{1}{U_{h2}} = \frac{1}{\alpha_1} + \frac{d_{h2}}{\lambda} + \frac{1}{\alpha_2}$
$Q_{h3} = U_{h3} A_{h3} (T_{s2} - T_{ENV})$
$Q_{h1} = Q_{HS}$
System s1
System s2
Environment
Q_{h2}
Q_{h3}
$\frac{dH_{s1}}{dt} = Q_{h1} - Q_{h2}$
$H_{s1} = m_{s1} c_{p,s1} T_{s1}$
$\frac{dH_{s2}}{dt} = Q_{h2} - Q_{h3}$
$H_{s2} = m_{s2} c_{p,s2} T_{s2}$
Automatically Generated by Mobatec Modeller
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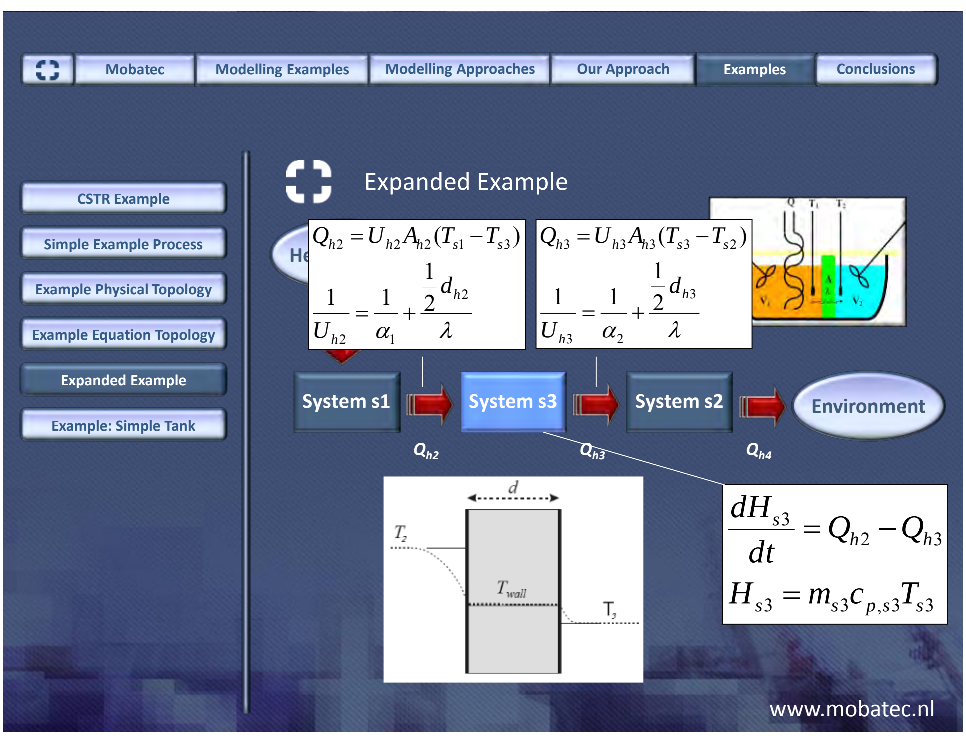
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Expanded Example
$Q_{h2} = U_{h2} A_{h2} (T_{s1} - T_{s3})$
$\frac{1}{U_{h2}} = \frac{1}{\alpha_1} + \frac{\frac{1}{2} d_{h2}}{\lambda}$
$Q_{h3} = U_{h3} A_{h3} (T_{s3} - T_{s2})$
$\frac{1}{U_{h3}} = \frac{1}{\alpha_2} + \frac{\frac{1}{2} d_{h3}}{\lambda}$
System s1
System s3
System s2
Environment
Q_{h2}
Q_{h3}
Q_{h4}
d
T_1
T_{wall}
T_2
$\frac{dH_{s3}}{dt} = Q_{h2} - Q_{h3}$
$H_{s3} = m_{s3} c_{p,s3} T_{s3}$
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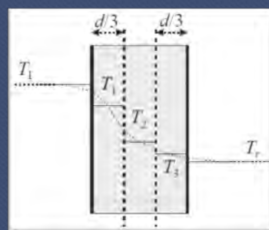
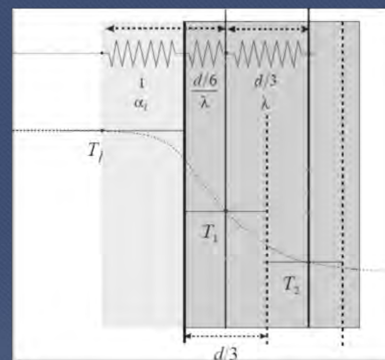
Expanded Example





$$U_1 = \frac{1}{\left(\frac{1}{\alpha_1} + \frac{d/6}{\lambda}\right)}$$

$$U_2 = \frac{\lambda}{d/3}$$

....

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